

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 18, 2023 – 09:46 AM EDT

PDB ID	:	2E93
Title	:	S. cerevisiae geranylgeranyl pyrophosphate synthase in complex with BPH-629
Authors	:	Guo, R.T.; Cao, R.; Ko, T.P.; Chen, C.KM.; Jeng, W.Y.; Chang, T.H.;
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Deposited on	:	2007-01-24
Resolution	:	2.12  Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

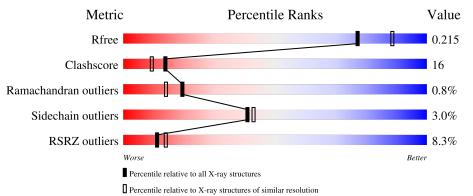
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	$6241 \ (2.14-2.10)$
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain			
1	А	340	70%	16%	·	12%
1	В	340	68%	21%		• 8%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5652 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	299	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	299	2442	1569	414	450	9	0	0	0
1	В	314	Total	С	Ν	0	S	0	0	0
	D		2571	1652	432	477	10	0	0	0

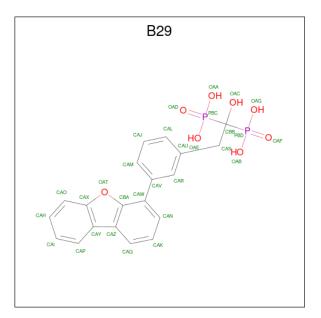
• Molecule 1 is a protein called Geranylgeranyl pyrophosphate synthetase.

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	cloning artifact	UNP Q12051
А	2	THR	-	cloning artifact	UNP Q12051
А	3	LYS	-	cloning artifact	UNP Q12051
А	4	ASN	-	cloning artifact	UNP Q12051
А	5	LYS	-	cloning artifact	UNP Q12051
В	1	MET	-	cloning artifact	UNP Q12051
В	2	THR	-	cloning artifact	UNP Q12051
В	3	LYS	-	cloning artifact	UNP Q12051
В	4	ASN	-	cloning artifact	UNP Q12051
В	5	LYS	_	cloning artifact	UNP Q12051

There are 10 discrepancies between the modelled and reference sequences:

• Molecule 2 is [2-(3-DIBENZOFURAN-4-YL-PHENYL)-1-HYDROXY-1-PHOSPHONO-ET HYL]-PHOSPHONIC ACID (three-letter code: B29) (formula:  $C_{20}H_{18}O_8P_2$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	Δ	1	Total	С	0	Р	0	0
	Л	T	30	20	8	2	0	0
2	Δ	1	Total	С	Ο	Р	0	0
	Л	1	30	20	8	2	0	0
2	В	1	Total	С	Ο	Р	0	0
	D	1	30	20	8	2	0	0
2	В	1	Total	С	0	Р	0	0
	D	I	30	20	8	2	0	0

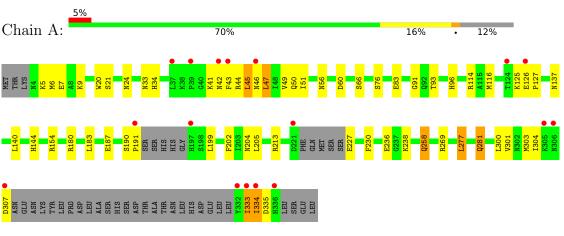
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	280	Total         O           280         280	0	0
3	В	239	Total         O           239         239	0	0



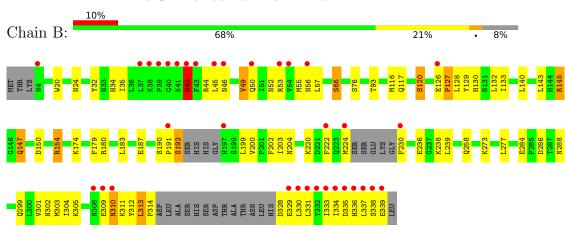
## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Geranyl geranyl pyrophosphate synthetase

• Molecule 1: Geranylgeranyl pyrophosphate synthetase





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	45.79Å 115.82Å 130.00Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	28.96 - 2.12	Depositor
Resolution (A)	28.96 - 2.12	EDS
% Data completeness	93.6 (28.96-2.12)	Depositor
(in resolution range)	94.1 (28.96-2.12)	EDS
R <sub>merge</sub>	0.04	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.11 (at 2.12 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
D D.	0.167 , $0.217$	Depositor
$R, R_{free}$	0.165 , $0.215$	DCC
$R_{free}$ test set	1873 reflections $(4.98\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	26.2	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36, 63.7	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5652	wwPDB-VP
Average B, all atoms $(Å^2)$	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:  $\mathbf{B29}$ 

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.90	1/2485~(0.0%)	0.88	4/3362~(0.1%)	
1	В	0.87	0/2617	0.83	3/3542~(0.1%)	
All	All	0.88	1/5102~(0.0%)	0.86	7/6904~(0.1%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	236	GLU	CB-CG	5.06	1.61	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	269	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	А	60	ASP	CB-CG-OD1	8.07	125.57	118.30
1	А	269	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	В	145	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	В	150	ASP	CB-CG-OD1	5.59	123.33	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2442	0	2494	73	0
1	В	2571	0	2615	96	0
2	А	60	0	28	6	0
2	В	60	0	28	9	0
3	А	280	0	0	12	0
3	В	239	0	0	8	0
All	All	5652	0	5165	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 163 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ILE:HG21	1:B:334:ILE:HD13	1.28	1.14
1:B:126:GLU:HG3	3:B:1089:HOH:O	1.69	0.92
1:B:258:GLN:HG2	1:B:286:ASP:OD2	1.69	0.91
1:B:52:ASN:HD21	1:B:57:LEU:H	1.12	0.89
1:A:258:GLN:HE21	1:A:258:GLN:H	1.16	0.89

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	291/340~(86%)	282~(97%)	7~(2%)	2(1%)	22 17
1	В	306/340~(90%)	299~(98%)	4 (1%)	3~(1%)	15 10
All	All	597/680~(88%)	581 (97%)	11 (2%)	5(1%)	19 14

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	334	ILE
1	В	42	ASN
1	В	310	ASN
1	В	127	PRO
1	А	333	ILE

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	279/317~(88%)	273~(98%)	6~(2%)	52 55		
1	В	295/317~(93%)	284 (96%)	11 (4%)	34 34		
All	All	574/634~(90%)	557~(97%)	17 (3%)	41 43		

 $5~{\rm of}~17$  residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	313	LEU
1	В	336	HIS
1	В	49	VAL
1	В	66	SER
1	В	120	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	24	ASN
1	В	299	GLN
1	В	52	ASN
1	В	204	ASN
1	В	42	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.



#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Mol Type Chain		Res	Link	Link Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	B29	В	904	-	29,33,33	2.54	9 (31%)	39,52,52	1.31	5 (12%)
2	B29	В	903	-	29,33,33	2.55	9 (31%)	39,52,52	1.28	4 (10%)
2	B29	А	902	-	29,33,33	2.55	9 (31%)	39,52,52	1.50	10 (25%)
2	B29	А	901	-	29,33,33	2.53	9 (31%)	39,52,52	1.27	6 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B29	В	904	-	-	1/23/27/27	0/4/4/4
2	B29	В	903	-	-	1/23/27/27	0/4/4/4
2	B29	А	902	-	-	3/23/27/27	0/4/4/4
2	B29	А	901	-	-	3/23/27/27	0/4/4/4

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	903	B29	PBC-OAD	7.04	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	902	B29	PBD-OAF	6.93	1.61	1.50
2	В	904	B29	PBC-OAD	6.86	1.61	1.50
2	В	904	B29	PBD-OAF	6.85	1.61	1.50
2	В	903	B29	PBD-OAF	6.82	1.61	1.50

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The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	904	B29	OAG-PBD-OAF	-3.85	104.41	113.06
2	А	902	B29	OAE-PBC-OAD	-3.62	104.94	113.06
2	А	902	B29	PBD-CBB-PBC	-3.49	106.56	112.81
2	А	901	B29	OAB-PBD-CBB	3.36	113.69	106.17
2	В	903	B29	CAN-CAW-CBA	3.33	120.36	116.50

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	902	B29	CAU-CAS-CBB-PBC
2	А	902	B29	CAU-CAS-CBB-PBD
2	А	902	B29	CAU-CAS-CBB-OAC
2	А	901	B29	CBB-CAS-CAU-CAR
2	А	901	B29	CBB-CAS-CAU-CAL

There are no ring outliers.

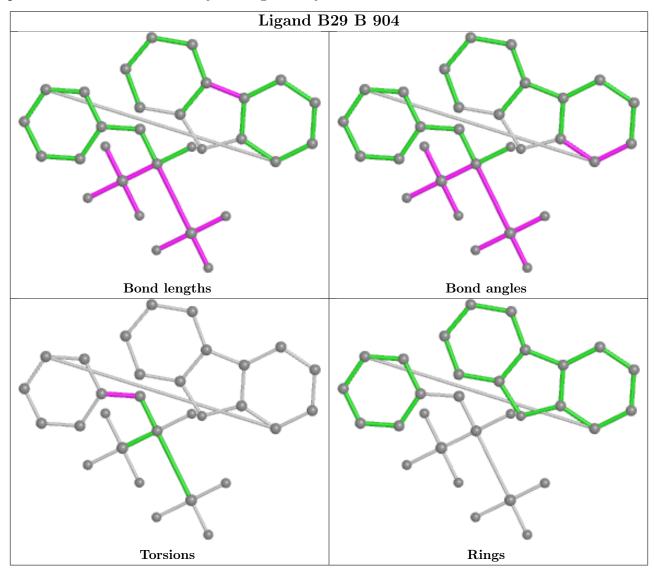
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	904	B29	6	0
2	В	903	B29	4	0
2	А	902	B29	4	0
2	А	901	B29	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

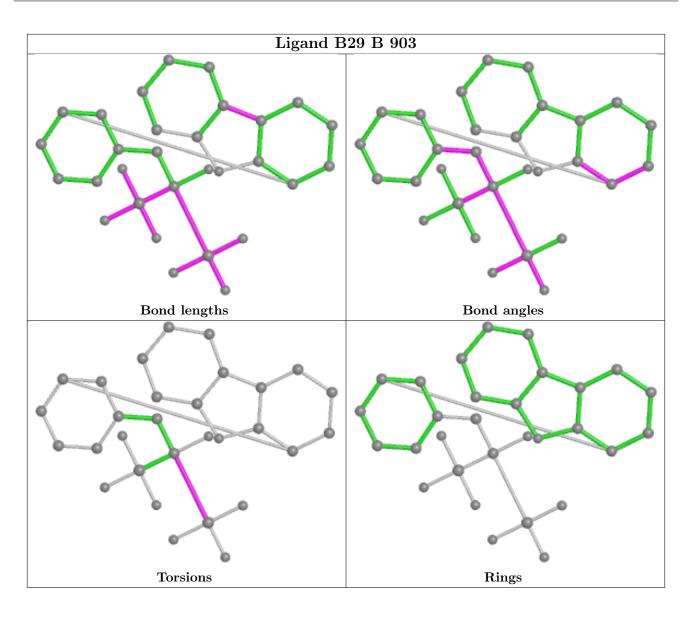


any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



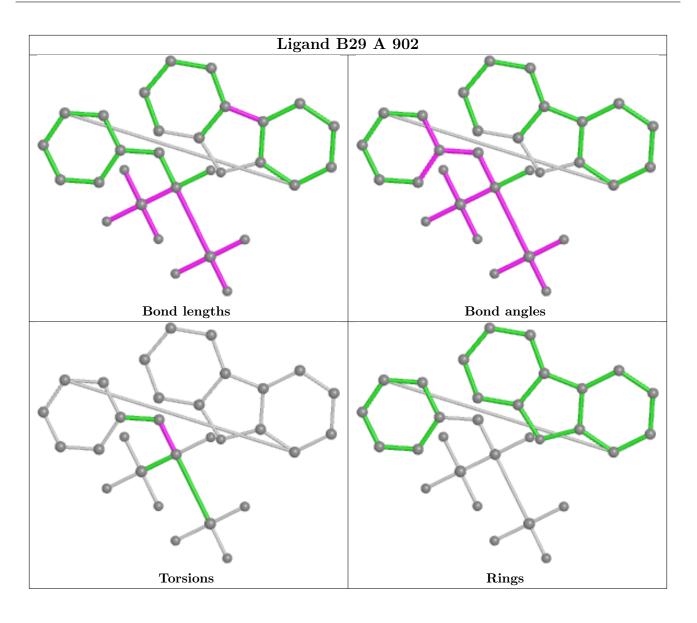






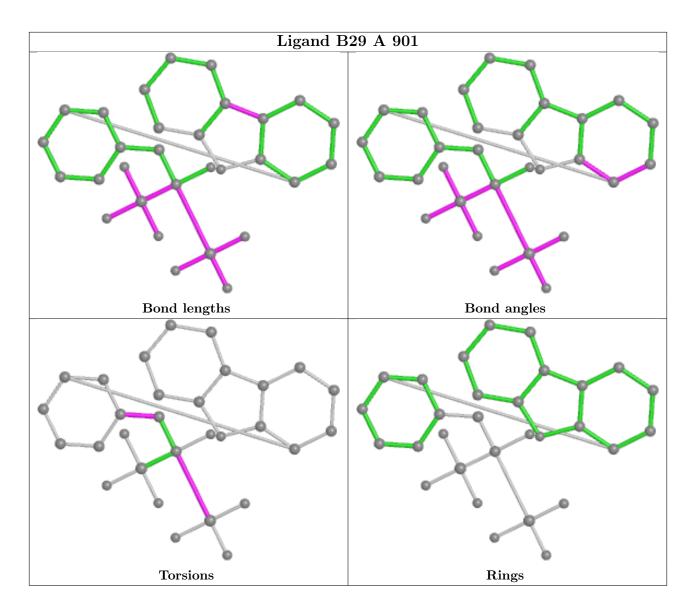












#### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	299/340~(87%)	0.11	17 (5%) 23 28	17, 27, 59, 102	0
1	В	314/340~(92%)	0.28	34 (10%) 5 7	17, 31, 78, 99	0
All	All	613/680~(90%)	0.20	51 (8%) 11 14	17, 29, 67, 102	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	43	PHE	7.5
1	В	332	TYR	6.8
1	В	43	PHE	6.6
1	А	46	ASN	5.6
1	В	197	HIS	5.4

### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

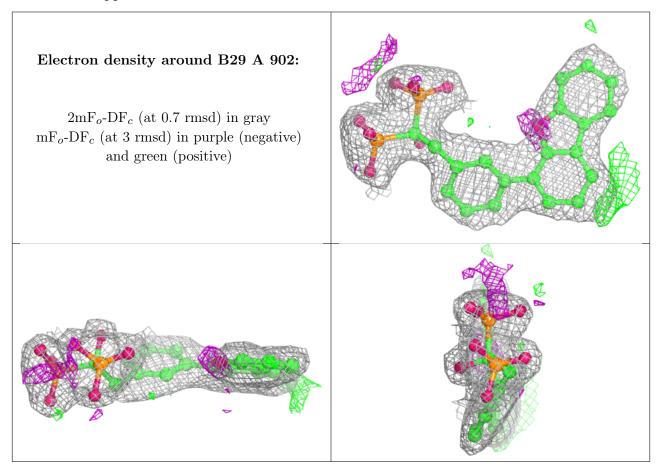
### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

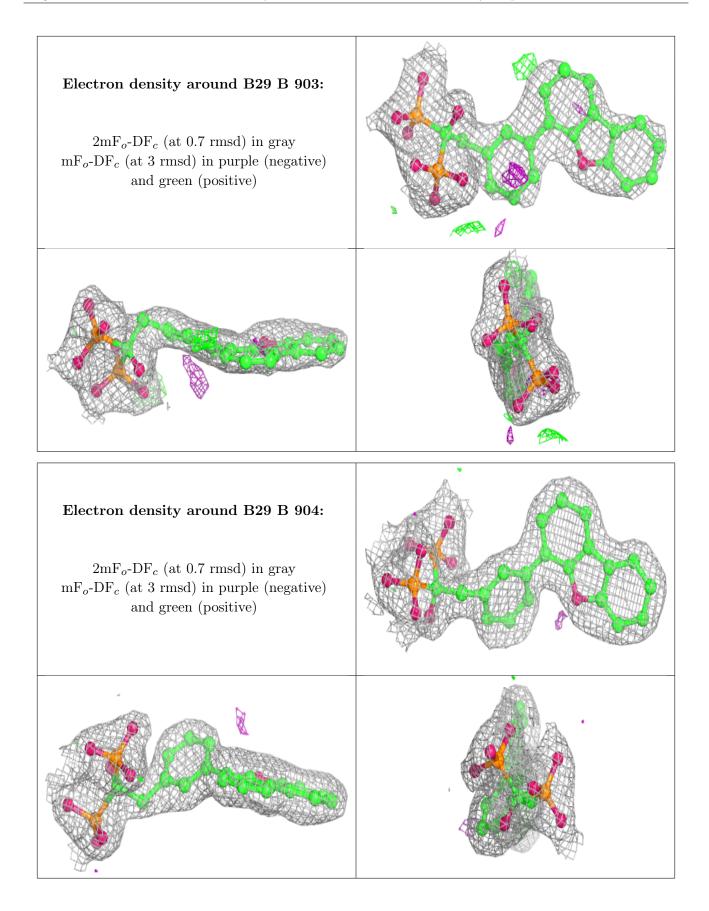


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	B29	А	902	30/30	0.94	0.13	31,37,44,46	0
2	B29	В	903	30/30	0.95	0.13	34,50,55,56	0
2	B29	В	904	30/30	0.96	0.12	26,30,36,37	0
2	B29	А	901	30/30	0.97	0.12	24,27,30,32	0

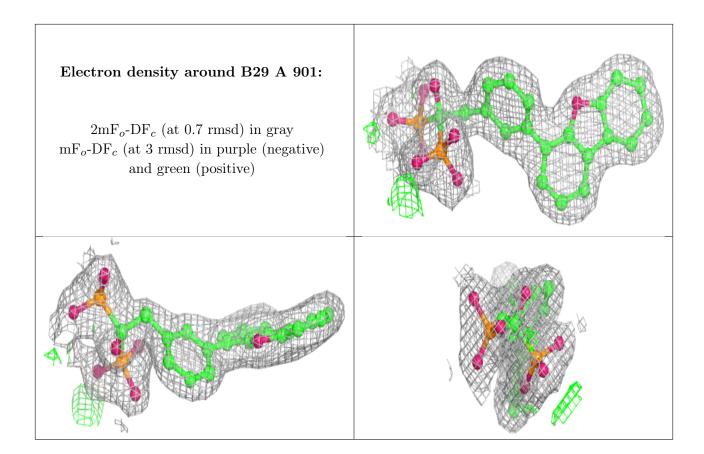
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











### 6.5 Other polymers (i)

There are no such residues in this entry.

